

Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 12:20 PM JST

PDB ID	:	8JZG
Title	:	C. glutamicum S-adenosylmethionine synthase co-crystallized with Adenosine,
		triphosphate, and SAM
Authors	:	Lee, S.; Kim, K.J.
Deposited on	:	2023-07-05
Resolution	:	2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	407	7%	19%	• 5%
1	В	407	8%	21%	•••
1	С	407	69%	23%	• 5%
1	D	407	9%	20%	• 5%



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12405 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	205	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	300	2948	1848	517	576	$\overline{7}$	0	0	0
1	Р	200	Total	С	Ν	0	S	0	0	0
	D	390	2984	1869	523	585	$\overline{7}$	0	0	0
1	C	286	Total	С	Ν	0	S	0	0	0
		380	2957	1853	518	579	$\overline{7}$	0	0	0
1	П	297	Total	С	Ν	0	S	0	0	0
	387	2964	1858	519	580	$\overline{7}$	0	0	0	

• Molecule 1 is a protein called S-adenosylmethionine synthase.

• Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Δ	1	Total	С	Ν	0	0	0	
2	11	1	19	10	5	4	0	0	
2	В	1	Total	С	Ν	Ο	0	0	
	D	1	19	10	5	4	0	0	



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	С	1	Total	С	Ν	Ο	0	0
Z	U	1	19	10	5	4	0	0
9	Л	1	Total	С	Ν	0	0	0
Z	D	1	19	10	5	4	0	0

• Molecule 3 is TRIPHOSPHATE (three-letter code: 3PO) (formula: $H_5O_{10}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	۸	1	Total O P	0	0
0	Л	1	13 10 3	0	0
3	В	1	Total O P	0	0
0	D	1	13 10 3	0	0
2	С	1	Total O P	0	0
0	U	1	13 10 3	0	0
3	Л	1	Total O P	0	0
J	D	1	13 10 3	0	0

• Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf	
4	Λ	1	Total	С	Ν	0	\mathbf{S}	0	0
4	Л	1	27	15	6	5	1	0	0
4	В	1	Total	С	Ν	0	\mathbf{S}	0	0
4	D	1	27	15	6	5	1	0	0
4	С	1	Total	С	Ν	Ο	\mathbf{S}	0	0
4	U	1	27	15	6	5	1	0	0
4	П	1	Total	С	Ν	Ο	S	0	0
4			27	15	6	5	1	0	U





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	А	1	Total 9	0 7	Р 2	0	0

• Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	2	Total Mg 2 2	0	0
7	В	2	Total Mg 2 2	0	0
7	С	2	Total Mg 2 2	0	0
7	D	2	Total Mg 2 2	0	0

• Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	2	Total K 2 2	0	0
8	С	1	Total K 1 1	0	0
8	D	1	Total K 1 1	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	92	Total O 92 92	0	0
9	В	91	Total O 91 91	0	0
9	С	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	0	0
9	D	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: S-adenosylmethionine synthase





• Molecule 1: S-adenosylmethionine synthase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	61.31Å 116.81Å 116.31Å	Deperitor
a, b, c, α , β , γ	90.00° 103.31° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	32.63 - 2.39	Depositor
Resolution (A)	32.61 - 2.39	EDS
% Data completeness	98.9 (32.63-2.39)	Depositor
(in resolution range)	98.9(32.61-2.39)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.194 , 0.260	Depositor
Π, Π_{free}	0.198 , 0.268	DCC
R_{free} test set	3194 reflections $(5.13%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	34.8	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.36 , 45.4	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12405	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, 3PO, ADN, POP, GOL, SAM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond lengths		Bond angles	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.73	0/3000	0.88	0/4075
1	В	0.64	0/3036	0.79	0/4124
1	С	0.71	0/3009	0.87	2/4087~(0.0%)
1	D	0.71	0/3016	0.85	0/4097
All	All	0.69	0/12061	0.85	2/16383~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	102	GLU	N-CA-C	-6.02	94.75	111.00
1	С	264	ARG	NE-CZ-NH1	6.00	123.30	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2948	0	2917	65	1
1	В	2984	0	2944	70	0
1	С	2957	0	2923	67	1
1	D	2964	0	2932	67	0
2	А	19	0	13	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	19	0	13	0	0
2	С	19	0	13	1	0
2	D	19	0	13	1	0
3	А	13	0	0	0	0
3	В	13	0	0	1	0
3	С	13	0	0	0	0
3	D	13	0	0	0	0
4	А	27	0	22	1	0
4	В	27	0	22	1	0
4	С	27	0	22	0	0
4	D	27	0	22	4	0
5	А	6	0	8	0	0
5	В	6	0	8	0	0
6	А	9	0	0	2	0
7	А	2	0	0	0	0
7	В	2	0	0	0	0
7	С	2	0	0	0	0
7	D	2	0	0	0	0
8	А	2	0	0	0	0
8	С	1	0	0	0	0
8	D	1	0	0	0	0
9	А	92	0	0	1	0
9	В	91	0	0	2	0
9	С	55	0	0	0	0
9	D	45	0	0	1	0
All	All	12405	0	11872	251	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:D:50:VAL:HG12	1:D:255:PRO:HB3	1.44	0.99
1:D:260:GLY:C	1:D:261:LEU:HD23	1.90	0.91
1:B:333:GLU:OE2	9:B:601:HOH:O	1.91	0.88
1:C:61:VAL:O	1:C:102:GLU:O	1.91	0.87
1:C:63:THR:HG22	1:C:65:ALA:H	1.39	0.86
1:D:50:VAL:CG1	1:D:255:PRO:HB3	2.06	0.85
1:D:48:THR:H	1:D:262:THR:HG23	1.44	0.82
1:D:358:ARG:HH11	1:D:358:ARG:HG3	1.48	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:11:THR:HG22	1:B:136:LEU:HD12	1.69	0.73
1:B:89:PHE:CD1	1:B:255:PRO:HG2	2.23	0.73
1:D:28:SER:OG	1:D:262:THR:HG21	1.89	0.71
1:B:127:ASP:HA	1:B:360:ALA:HB3	1.73	0.71
1:C:188:ASP:HB2	1:C:192:ARG:HG3	1.72	0.71
1:B:136:LEU:HD22	1:B:136:LEU:H	1.56	0.71
1:D:261:LEU:HD23	1:D:261:LEU:N	2.04	0.71
1:D:363:ILE:HA	1:D:368:LEU:HD12	1.72	0.71
1:A:299:ARG:HG3	1:A:382:PHE:CD1	2.27	0.69
1:D:358:ARG:HH11	1:D:358:ARG:CG	2.06	0.68
1:A:190:GLN:HB2	1:A:192:ARG:HD3	1.76	0.68
1:C:266:ILE:HD11	1:D:266:ILE:HD11	1.74	0.68
1:A:51:THR:HG22	1:A:54:ILE:HG23	1.76	0.68
1:D:48:THR:H	1:D:262:THR:CG2	2.05	0.68
1:C:68:GLU:H	1:C:68:GLU:CD	1.98	0.68
1:C:154:ALA:O	1:C:158:ARG:HG3	1.95	0.66
1:C:182:GLN:HB3	1:C:200:VAL:HG13	1.76	0.65
1:A:397:VAL:O	1:A:401:ARG:HG3	1.98	0.64
1:A:56:HIS:CE1	6:A:505:POP:O1	2.50	0.63
1:C:286:ASP:OD1	1:C:288:SER:OG	2.11	0.63
1:A:88:GLY:O	1:A:256:MET:HG3	1.99	0.63
1:C:142:THR:OG1	1:C:144:GLU:HG3	1.99	0.63
1:A:57:VAL:HG12	1:A:100:ILE:HD11	1.80	0.62
1:C:204:GLN:HA	1:C:250:PHE:O	1.98	0.62
1:C:196:LEU:HD21	1:C:199:VAL:HG12	1.80	0.62
1:C:308:ALA:HB3	1:C:310:LEU:HG	1.83	0.61
1:B:404:LEU:O	1:B:406:LEU:HG	2.01	0.61
1:D:227:ILE:HG23	1:D:232:ILE:HG13	1.82	0.61
1:A:401:ARG:HB3	1:A:401:ARG:NH1	2.15	0.60
1:A:49:VAL:HG13	1:A:261:LEU:HD23	1.82	0.60
1:D:74:ARG:HD3	1:D:91:GLY:O	2.02	0.60
1:B:396:ARG:O	1:B:399:GLU:HG2	2.01	0.60
1:D:143:ASN:ND2	1:D:312:ASP:OD1	2.35	0.60
1:D:252:LEU:HD13	1:D:256:MET:HG3	1.82	0.60
1:D:276:ARG:NH1	1:D:315:GLU:OE1	2.32	0.60
1:B:356:ASP:OD1	1:B:358:ARG:HD3	2.02	0.59
1:A:74:ARG:NH1	1:A:94:CYS:O	2.33	0.59
1:A:63:THR:HG22	4:A:503:SAM:H3'	1.85	0.59
1:C:298:MET:HG3	1:C:316:VAL:HB	1.84	0.59
1:A:401:ARG:HB3	1:A:401:ARG:HH11	1.67	0.58
1:B:43:ARG:NH1	1:B:124:GLU:HG2	2.18	0.58



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:325:ALA:HB1	1:D:358:ARG:HD2	1.86	0.57
1:A:379:TYR:O	1:A:384:ARG:HD3	2.04	0.57
1:A:188:ASP:OD2	1:A:192:ARG:HB2	2.04	0.57
1:D:298:MET:HA	1:D:298:MET:CE	2.35	0.57
1:A:247:SER:HB2	1:B:323:GLY:HA3	1.87	0.57
1:C:142:THR:O	1:C:148:TYR:HA	2.05	0.56
1:B:103:GLN:HB3	4:B:503:SAM:H4'	1.87	0.56
1:B:137:MET:CE	1:B:318:VAL:HG13	2.35	0.56
1:D:9:LEU:HD23	1:D:186:ALA:HA	1.88	0.56
1:B:142:THR:O	1:B:148:TYR:HA	2.06	0.55
1:D:384:ARG:HG2	1:D:387:LEU:HD12	1.88	0.55
1:C:264:ARG:NH2	1:D:47:GLU:OE2	2.39	0.55
1:B:70:PRO:O	1:B:74:ARG:HG3	2.07	0.55
1:B:282:PHE:HA	1:B:292:ARG:HG3	1.88	0.55
1:C:188:ASP:OD1	1:C:194:SER:HB2	2.07	0.55
1:C:150:PRO:HB3	1:C:274:MET:HG3	1.89	0.54
1:B:127:ASP:OD2	1:B:364:ARG:NH2	2.41	0.54
1:B:333:GLU:OE1	1:B:335:PHE:N	2.32	0.54
1:C:35:LEU:HD22	1:C:63:THR:HG21	1.90	0.54
1:B:123:VAL:HG22	1:B:129:ALA:CB	2.38	0.53
1:C:47:GLU:HG3	1:D:261:LEU:HD11	1.90	0.53
1:D:84:SER:OG	1:D:86:GLU:HB2	2.08	0.53
1:C:367:ASP:O	1:C:370:ARG:HD3	2.09	0.53
1:D:298:MET:HA	1:D:298:MET:HE2	1.91	0.53
1:D:308:ALA:HA	1:D:397:VAL:HG13	1.90	0.53
1:A:367:ASP:O	1:A:370:ARG:HD3	2.08	0.53
1:B:367:ASP:O	1:B:370:ARG:NH1	2.41	0.53
1:D:270:THR:HG21	1:D:277:HIS:CD2	2.43	0.53
1:C:51:THR:HG21	1:D:58:VAL:HG13	1.91	0.52
1:D:358:ARG:HG3	1:D:358:ARG:NH1	2.21	0.52
1:A:299:ARG:NH1	1:A:392:GLU:OE1	2.43	0.52
1:C:125:GLU:HA	1:C:128:ARG:HB3	1.89	0.52
1:D:312:ASP:HB2	1:D:337:THR:HB	1.91	0.52
1:C:286:ASP:OD2	1:C:289:LYS:NZ	2.42	0.52
1:D:164:THR:HG21	1:D:379:TYR:OH	2.08	0.52
1:D:243:LEU:HB3	1:D:246:PRO:HG3	1.92	0.51
1:A:396:ARG:O	1:A:399:GLU:HG2	2.10	0.51
1:B:252:LEU:HD13	1:B:256:MET:CE	2.40	0.51
1:A:47:GLU:HG3	1:B:261:LEU:HD11	1.92	0.51
1:C:137:MET:SD	1:C:137:MET:N	2.84	0.51
1:D:59:GLY:O	1:D:100:ILE:HA	2.10	0.51



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:299:ARG:HD2	1:B:299:ARG:O	2.11	0.51	
1:A:3:GLN:N	1:A:4:PRO:CD	2.74	0.51	
1:C:397:VAL:O	1:C:401:ARG:HG2	2.10	0.51	
1:D:399:GLU:CD	1:D:399:GLU:H	2.13	0.51	
1:B:49:VAL:HG13	1:B:261:LEU:CD2	2.41	0.50	
1:D:347:ILE:O	1:D:351:VAL:HG23	2.11	0.50	
1:B:9:LEU:HD23	1:B:186:ALA:HA	1.93	0.50	
1:A:56:HIS:ND1	6:A:505:POP:O1	2.44	0.50	
1:A:261:LEU:HD11	1:B:47:GLU:CG	2.41	0.50	
1:B:342:LEU:HA	1:B:346:GLN:OE1	2.11	0.50	
1:C:127:ASP:HB3	1:C:358:ARG:CZ	2.41	0.50	
1:B:292:ARG:HD3	1:B:296:TYR:CZ	2.47	0.50	
1:B:308:ALA:HA	1:B:401:ARG:HH21	1.76	0.50	
1:C:401:ARG:NH1	1:C:406:LEU:HD13	2.27	0.50	
1:D:80:ILE:O	1:D:167:ARG:NH1	2.45	0.50	
1:D:88:GLY:O	1:D:256:MET:HG2	2.12	0.49	
1:D:355:PHE:CE1	1:D:396:ARG:HG2	2.47	0.49	
1:B:49:VAL:HG13	1:B:261:LEU:HD21	1.93	0.49	
1:D:20:PRO:HA	1:D:23:ILE:HD12	1.94	0.49	
1:A:261:LEU:HD11	1:B:47:GLU:HG2	1.93	0.49	
1:C:136:LEU:O	1:C:278:GLY:HA3	2.13	0.49	
1:B:50:VAL:HG12	1:B:55:VAL:HG22	1.94	0.49	
1:B:212:ALA:O	1:B:216:THR:HG23	2.13	0.49	
1:A:142:THR:O	1:A:148:TYR:HA	2.12	0.49	
1:A:199:VAL:HG11	1:A:223:ILE:HD13	1.95	0.49	
1:A:143:ASN:ND2	1:A:312:ASP:OD1	2.46	0.49	
1:C:298:MET:HA	1:C:298:MET:HE2	1.95	0.48	
1:A:142:THR:OG1	1:A:144:GLU:HG3	2.13	0.48	
1:B:136:LEU:HD22	1:B:136:LEU:N	2.25	0.48	
1:B:136:LEU:N	1:B:136:LEU:HD13	2.28	0.48	
1:A:2:ALA:HA	1:B:405:LYS:HD2	1.96	0.48	
1:B:396:ARG:HG3	1:B:399:GLU:HG3	1.95	0.48	
1:D:89:PHE:CD2	1:D:255:PRO:HG2	2.48	0.48	
1:C:203:THR:O	1:C:250:PHE:HB3	2.14	0.48	
1:B:394:ILE:O	1:B:394:ILE:HG22	2.14	0.48	
1:D:149:MET:CG	1:D:383:GLY:HA3	2.43	0.48	
1:C:296:TYR:CE2	1:C:391:TRP:CH2	3.01	0.48	
1:D:100:ILE:HD11	4:D:503:SAM:N7	2.29	0.48	
1:C:166:VAL:HG13	1:C:172:VAL:HB	1.96	0.47	
1:A:401:ARG:NH1	1:A:407:ALA:O	2.47	0.47	
1:B:292:ARG:HD3	1:B:296:TYR:OH	2.14	0.47	



	i agein	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:266:ILE:HD11	1:B:266:ILE:HD11	1.96	0.47	
1:C:188:ASP:HB2	1:C:192:ARG:CG	2.41	0.47	
1:A:49:VAL:HG13	1:A:261:LEU:CD2	2.44	0.47	
1:B:282:PHE:CA	1:B:292:ARG:HG3	2.44	0.47	
1:D:8:ARG:NH2	1:D:191:ASP:OD1	2.40	0.47	
1:B:123:VAL:HG22	1:B:129:ALA:HB1	1.96	0.47	
1:D:245:ASN:N	1:D:246:PRO:HD3	2.30	0.47	
1:D:161:ARG:NH1	1:D:386:ASP:OD2	2.48	0.46	
1:B:138:PHE:CE1	1:B:317:GLN:HB2	2.50	0.46	
1:A:51:THR:HG22	1:A:54:ILE:CG2	2.43	0.46	
1:C:51:THR:HG21	1:D:58:VAL:CG1	2.45	0.46	
1:C:308:ALA:HA	1:C:397:VAL:HG13	1.97	0.46	
1:D:89:PHE:CD2	1:D:255:PRO:CG	2.98	0.46	
1:A:135:GLY:O	1:A:319:ALA:HA	2.16	0.46	
1:B:270:THR:HG21	1:B:277:HIS:CD2	2.51	0.46	
1:D:143:ASN:ND2	1:D:312:ASP:HA	2.31	0.46	
1:B:124:GLU:HA	9:B:668:HOH:O	2.16	0.46	
1:A:394:ILE:HG12	9:A:648:HOH:O	2.16	0.46	
1:A:347:ILE:O	1:A:350:ALA:HB3	2.15	0.45	
1:B:126:ASP:OD1	1:B:126:ASP:N	2.49	0.45	
1:B:127:ASP:HA	1:B:360:ALA:CB	2.45	0.45	
1:C:101:GLY:O	1:C:102:GLU:HB2	2.16	0.45	
1:C:270:THR:HG21	1:C:277:HIS:CD2	2.51	0.45	
1:C:296:TYR:CD2	1:C:391:TRP:CZ3	3.04	0.45	
1:A:66:TYR:CE2	4:D:503:SAM:HE2	2.51	0.45	
1:D:54:ILE:HD12	1:D:95:GLY:C	2.37	0.45	
1:A:379:TYR:O	1:A:384:ARG:NH1	2.49	0.45	
1:A:322:ILE:HG12	1:B:247:SER:CB	2.46	0.45	
1:C:258:ASP:OD2	2:C:501:ADN:H5'1	2.16	0.45	
1:C:269:ASP:HB3	1:C:381:HIS:CD2	2.51	0.45	
1:A:50:VAL:HG12	1:A:55:VAL:HG22	1.99	0.45	
1:C:70:PRO:O	1:C:74:ARG:HG3	2.17	0.45	
1:D:261:LEU:N	1:D:261:LEU:CD2	2.76	0.45	
1:A:47:GLU:CG	1:B:261:LEU:HD11	2.47	0.45	
1:C:297:ALA:O	1:C:300:TRP:HB3	2.17	0.45	
1:D:334:THR:OG1	1:D:344:ASP:OD1	2.35	0.45	
1:A:43:ARG:HB2	1:A:62:ARG:HB3	1.99	0.45	
1:A:145:THR:HB	1:A:147:GLU:OE2	2.17	0.45	
1:D:140:TYR:CE2	1:D:150:PRO:HG3	2.52	0.45	
1:D:276:ARG:HD3	1:D:315:GLU:OE2	2.16	0.45	
1:B:137:MET:HE2	1:B:318:VAL:HG13	1.98	0.44	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:276:ARG:HD3	1:C:315:GLU:OE1	2.18	0.44	
1:A:215:GLU:HA	1:A:244:ILE:HD12	1.98	0.44	
1:B:57:VAL:HG12	1:B:100:ILE:HD11	2.00	0.44	
1:B:266:ILE:HD12	1:B:277:HIS:CE1	2.52	0.44	
1:D:296:TYR:CD2	1:D:391:TRP:CZ3	3.05	0.44	
1:C:59:GLY:O	1:C:100:ILE:HA	2.18	0.44	
1:C:153:ILE:HG13	1:C:157:HIS:CD2	2.53	0.44	
1:D:78:ILE:HD11	1:D:92:ARG:HG3	2.00	0.44	
1:A:98:VAL:HG13	1:A:100:ILE:HD13	2.00	0.44	
1:C:15:VAL:HG23	1:C:22:LYS:HG3	1.99	0.44	
1:A:74:ARG:O	1:A:78:ILE:HG13	2.18	0.43	
1:A:311:ALA:HB1	1:A:337:THR:OG1	2.18	0.43	
1:D:69:ILE:N	1:D:70:PRO:CD	2.81	0.43	
1:A:354:VAL:HG21	1:A:400:LEU:HD23	2.00	0.43	
1:D:149:MET:HG3	1:D:383:GLY:HA3	2.00	0.43	
1:D:161:ARG:HG2	1:D:379:TYR:CG	2.53	0.43	
1:A:190:GLN:HB2	1:A:192:ARG:CD	2.47	0.43	
1:A:264:ARG:NH2	1:B:262:THR:O	2.49	0.43	
1:C:22:LYS:HD3	1:C:377:ALA:O	2.18	0.43	
1:D:260:GLY:O	1:D:261:LEU:HD23	2.14	0.43	
1:B:347:ILE:O	1:B:351:VAL:HG23	2.18	0.43	
1:C:128:ARG:HD3	1:C:128:ARG:HA	1.77	0.43	
1:A:155:LEU:HD12	1:A:185:PHE:CE2	2.53	0.43	
1:C:360:ALA:O	1:C:364:ARG:HG3	2.18	0.43	
1:D:298:MET:SD	1:D:318:VAL:HB	2.58	0.43	
1:A:369:LEU:O	1:A:370:ARG:HG3	2.19	0.43	
1:C:43:ARG:O	1:C:61:VAL:HA	2.18	0.43	
1:A:280:GLY:HA2	3:B:502:3PO:O1G	2.19	0.43	
1:C:215:GLU:HG2	1:C:244:ILE:HB	2.01	0.43	
1:C:298:MET:HG2	1:C:316:VAL:O	2.18	0.43	
1:C:151:LEU:HD11	1:C:232:ILE:HD11	2.01	0.42	
1:A:13:GLU:HG2	1:B:136:LEU:HD21	2.02	0.42	
1:A:188:ASP:OD1	1:A:190:GLN:HG2	2.18	0.42	
1:D:77:LEU:HD13	1:D:89:PHE:HE1	1.84	0.42	
1:B:135:GLY:C	1:B:136:LEU:HD13	2.40	0.42	
1:B:301:VAL:O	1:B:305:ILE:HG13	2.18	0.42	
1:A:204:GLN:HA	1:A:250:PHE:O	2.20	0.42	
1:D:297:ALA:O	1:D:300:TRP:HB3	2.19	0.42	
1:A:66:TYR:CD2	4:D:503:SAM:HE2	2.55	0.42	
1:C:54:ILE:HD12	1:C:95:GLY:C	2.40	0.42	
1:D:158:ARG:NH1	9:D:602:HOH:O	2.51	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:401:ARG:HH12	1:A:407:ALA:N	2.18	0.42	
1:B:387:LEU:HD12	1:B:389:LEU:HD11	2.02	0.42	
1:A:89:PHE:CE2	1:A:255:PRO:HG2	2.54	0.42	
1:B:24:CYS:SG	1:B:50:VAL:HG22	2.60	0.42	
1:C:334:THR:OG1	1:C:344:ASP:OD1	2.38	0.42	
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.96	0.42	
1:C:126:ASP:O	1:C:364:ARG:NH2	2.53	0.42	
1:B:252:LEU:HD13	1:B:256:MET:HE3	2.01	0.41	
1:C:137:MET:HG2	1:C:294:ALA:HB3	2.01	0.41	
1:A:215:GLU:HA	1:A:244:ILE:CD1	2.50	0.41	
1:B:103:GLN:O	1:B:104:SER:HB2	2.20	0.41	
1:D:258:ASP:OD2	2:D:501:ADN:H5'2	2.20	0.41	
1:B:252:LEU:HD13	1:B:256:MET:HE2	2.02	0.41	
1:A:369:LEU:C	1:A:370:ARG:HG3	2.41	0.41	
1:B:74:ARG:NH2	1:B:94:CYS:O	2.49	0.41	
1:C:347:ILE:O	1:C:350:ALA:HB3	2.20	0.41	
1:C:135:GLY:O	1:C:319:ALA:HA	2.21	0.41	
1:D:61:VAL:HG22	4:D:503:SAM:H2'	2.03	0.41	
1:D:286:ASP:OD1	1:D:288:SER:OG	2.15	0.41	
1:B:123:VAL:HG13	1:B:129:ALA:HB1	2.02	0.41	
1:C:290:VAL:HG22	1:C:294:ALA:HB2	2.03	0.41	
1:B:245:ASN:N	1:B:246:PRO:CD	2.84	0.41	
1:B:162:ARG:HG3	1:B:225:TRP:CE3	2.56	0.41	
1:C:49:VAL:HG13	1:C:261:LEU:CD2	2.50	0.41	
1:C:78:ILE:HD11	1:C:92:ARG:HG3	2.02	0.41	
1:B:93:THR:HG22	1:D:256:MET:HE2	2.03	0.41	
1:C:49:VAL:HG13	1:C:261:LEU:HD23	2.03	0.41	
1:A:47:GLU:HG3	1:B:261:LEU:CD1	2.50	0.40	
1:B:276:ARG:HD3	1:B:315:GLU:OE1	2.21	0.40	
1:C:298:MET:HA	1:C:298:MET:CE	2.51	0.40	
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.95	0.40	
1:A:214:LEU:O	1:A:218:LEU:HG	2.20	0.40	
1:C:145:THR:OG1	1:C:149:MET:N	2.44	0.40	
1:B:123:VAL:HG22	1:B:129:ALA:HB2	2.03	0.40	
1:B:164:THR:HG22	1:B:168:LYS:HD2	2.04	0.40	
1:C:127:ASP:OD1	1:C:364:ARG:NE	2.48	0.40	
1:C:216:THR:O	1:C:220:GLU:HG3	2.22	0.40	
1:D:8:ARG:HG3	1:D:8:ARG:HH11	1.86	0.40	

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:405:LYS:O	1:C:190:GLN:NE2[1_554]	1.77	0.43	

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	381/407~(94%)	366~(96%)	15~(4%)	0	100	100
1	В	386/407~(95%)	371~(96%)	15~(4%)	0	100	100
1	С	382/407~(94%)	357~(94%)	25~(6%)	0	100	100
1	D	383/407~(94%)	357~(93%)	26~(7%)	0	100	100
All	All	1532/1628~(94%)	1451 (95%)	81 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	310/328~(94%)	282 (91%)	28 (9%)	9 14
1	В	314/328~(96%)	291~(93%)	23~(7%)	14 22
1	С	311/328~(95%)	290~(93%)	21 (7%)	16 25
1	D	312/328~(95%)	293 (94%)	19 (6%)	18 30
All	All	1247/1312~(95%)	1156 (93%)	91 (7%)	14 22

All (91) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	7	VAL
1	А	22	LYS
1	А	47	GLU
1	А	51	THR
1	А	62	ARG
1	А	86	GLU
1	А	100	ILE
1	А	126	ASP
1	А	127	ASP
1	А	128	ARG
1	А	136	LEU
1	А	155	LEU
1	А	161	ARG
1	А	190	GLN
1	А	192	ARG
1	А	209	VAL
1	А	211	ARG
1	А	216	THR
1	А	250	PHE
1	А	256	MET
1	А	258	ASP
1	А	299	ARG
1	А	324	ARG
1	А	326	LYS
1	А	338	ASN
1	А	352	LEU
1	А	369	LEU
1	А	397	VAL
1	В	22	LYS
1	В	58	VAL
1	В	87	VAL
1	В	102	GLU
1	В	123	VAL
1	В	126	ASP
1	В	136	LEU
1	В	137	MET
1	В	161	ARG
1	В	162	ARG
1	В	190	GLN
1	В	208	GLU
1	В	250	PHE
1	В	258	ASP
1	В	289	LYS



Mol	Chain	Res	Type	
1	В	290	VAL	
1	В	292	ARG	
1	В	299	ARG	
1	В	324	ARG	
1	В	326	LYS	
1	В	336	ASP	
1	В	345	GLU	
1	В	396	ARG	
1	С	3	GLN	
1	С	13	GLU	
1	С	47	GLU	
1	С	60	GLU	
1	С	136	LEU	
1	С	137	MET	
1	С	151	LEU	
1	С	166	VAL	
1	С	167	ARG	
1	С	183	VAL	
1	С	199	VAL	
1	С	200	VAL	
1	С	234	ASP	
1	С	250	PHE	
1	С	258	ASP	
1	С	298	MET	
1	С	313	ARG	
1	С	324	ARG	
1	С	326	LYS	
1	С	345	GLU	
1	C	392	GLU	
1	D	8	ARG	
1	D	61	VAL	
1	D	86	GLU	
1	D	136	LEU	
1	D	137	MET	
1	D	147	GLU	
1	D	151	LEU	
1	D	161	ARG	
1	D	164	THR	
1	D	183	VAL	
1	D	215	GLU	
1	D	216	THR	
1	D	241	THR	



Continued from previous page...

Mol	Chain	Res	Type
1	D	250	PHE
1	D	256	MET
1	D	258	ASP
1	D	261	LEU
1	D	298	MET
1	D	358	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such side chains are listed below:

Mol	Chain	Res	Type
1	А	190	GLN
1	В	56	HIS
1	С	3	GLN
1	С	56	HIS
1	D	103	GLN
1	D	205	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SAM	А	503	-	24,29,29	0.79	2 (8%)	23,42,42	1.44	4 (17%)
3	3PO	А	502	7,8	8,12,12	1.13	1 (12%)	15,20,20	1.58	2 (13%)
6	POP	А	505	-	6,8,8	0.49	0	13,13,13	1.01	0
2	ADN	С	501	-	18,21,21	0.72	0	18,31,31	1.09	2 (11%)
2	ADN	D	501	-	18,21,21	0.62	0	18,31,31	0.84	1 (5%)
4	SAM	D	503	-	24,29,29	0.71	0	23,42,42	1.52	2 (8%)
5	GOL	В	504	-	$5,\!5,\!5$	0.11	0	$5,\!5,\!5$	0.32	0
2	ADN	А	501	-	18,21,21	0.70	0	18,31,31	0.78	1 (5%)
2	ADN	В	501	-	18,21,21	0.77	0	18,31,31	0.95	1 (5%)
5	GOL	А	504	-	$5,\!5,\!5$	0.10	0	$5,\!5,\!5$	0.47	0
3	3PO	С	502	7,8	8,12,12	1.05	0	15,20,20	2.03	5 (33%)
4	SAM	С	503	-	24,29,29	0.70	1 (4%)	23,42,42	1.26	3 (13%)
3	3PO	D	502	7	8,12,12	1.04	0	15,20,20	1.28	2 (13%)
3	3PO	В	502	7	8,12,12	1.46	1 (12%)	15,20,20	2.10	6 (40%)
4	SAM	В	503	-	24,29,29	0.73	1 (4%)	23,42,42	1.20	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	А	503	-	-	4/12/33/33	0/3/3/3
3	3PO	А	502	7,8	-	2/12/12/12	-
6	POP	А	505	-	-	0/6/6/6	-
2	ADN	С	501	-	-	0/2/22/22	0/3/3/3
2	ADN	D	501	-	-	2/2/22/22	0/3/3/3
4	SAM	D	503	-	-	2/12/33/33	0/3/3/3
5	GOL	В	504	-	-	2/4/4/4	-
2	ADN	А	501	-	-	0/2/22/22	0/3/3/3
2	ADN	В	501	-	-	0/2/22/22	0/3/3/3
5	GOL	А	504	-	-	2/4/4/4	-
3	3PO	С	502	7,8	-	1/12/12/12	-
4	SAM	С	503	-	-	2/12/33/33	0/3/3/3
3	3PO	D	502	7	-	1/12/12/12	-
3	3PO	В	502	7	-	0/12/12/12	-
4	SAM	В	503	-	-	$\frac{5/12}{33/33}$	0/3/3/3



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	503	SAM	OXT-C	-2.21	1.23	1.30
3	В	502	3PO	PG-O2G	-2.20	1.46	1.54
4	А	503	SAM	C8-N7	-2.19	1.30	1.34
4	С	503	SAM	OXT-C	-2.15	1.23	1.30
4	В	503	SAM	OXT-C	-2.12	1.23	1.30
3	А	502	3PO	PA-O5'	-2.01	1.47	1.54

All (6) bond length outliers are listed below:

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	503	SAM	OXT-C-O	-5.05	112.63	124.09
3	В	502	3PO	O2G-PG-O3B	4.43	119.47	104.64
3	С	502	3PO	O3G-PG-O3B	3.97	117.93	104.64
3	С	502	3PO	O2G-PG-O3B	3.86	117.58	104.64
3	С	502	3PO	PB-O3A-PA	-3.71	120.10	132.83
3	А	502	3PO	PB-O3A-PA	3.66	145.39	132.83
3	В	502	3PO	PB-O3A-PA	-3.53	120.70	132.83
3	В	502	3PO	PB-O3B-PG	3.47	144.72	132.83
4	С	503	SAM	OXT-C-O	-3.14	116.97	124.09
4	С	503	SAM	OXT-C-CA	3.08	123.88	113.38
4	А	503	SAM	O3'-C3'-C4'	-2.93	102.58	111.05
4	В	503	SAM	OXT-C-O	-2.89	117.53	124.09
4	А	503	SAM	O3'-C3'-C2'	2.69	120.52	111.82
2	В	501	ADN	C5-C6-N6	2.56	124.25	120.35
3	D	502	3PO	PB-O3B-PG	2.56	141.60	132.83
3	С	502	3PO	O3B-PG-O1G	-2.54	97.12	111.19
4	А	503	SAM	OXT-C-O	-2.52	118.37	124.09
3	С	502	3PO	PB-O3B-PG	2.50	141.41	132.83
4	D	503	SAM	OXT-C-CA	2.46	121.76	113.38
3	В	502	3PO	O3G-PG-O3B	2.43	112.78	104.64
4	А	503	SAM	O4'-C4'-C5'	2.42	114.99	108.88
4	В	503	SAM	C5-C6-N6	2.39	123.98	120.35
2	С	501	ADN	C5-C6-N6	2.30	123.85	120.35
2	D	501	ADN	C5-C6-N6	2.25	123.78	120.35
4	С	503	SAM	C3'-C2'-C1'	2.23	104.34	100.98
3	D	502	3PO	PB-O3A-PA	-2.19	125.33	132.83
3	Α	502	3PO	O2G-PG-O3B	2.16	111.88	104.64
3	В	502	3PO	O5'-PA-O3A	2.15	111.85	104.64
3	В	502	3PO	O3A-PA-O1A	-2.15	99.29	111.19
2	А	501	ADN	C5-C6-N6	2.12	123.57	120.35
2	С	501	ADN	C2'-C3'-C4'	2.07	106.67	102.64



There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
3	А	502	3PO	PB-O3A-PA-O2A
3	D	502	3PO	PB-O3B-PG-O2G
4	А	503	SAM	N-CA-CB-CG
4	А	503	SAM	O4'-C4'-C5'-SD
4	А	503	SAM	C3'-C4'-C5'-SD
4	В	503	SAM	O-C-CA-N
4	В	503	SAM	CB-CG-SD-CE
4	D	503	SAM	CB-CG-SD-CE
5	А	504	GOL	O1-C1-C2-C3
5	В	504	GOL	C1-C2-C3-O3
2	D	501	ADN	O4'-C4'-C5'-O5'
5	В	504	GOL	O2-C2-C3-O3
2	D	501	ADN	C3'-C4'-C5'-O5'
4	В	503	SAM	OXT-C-CA-N
4	С	503	SAM	OXT-C-CA-N
5	А	504	GOL	O1-C1-C2-O2
4	С	503	SAM	O-C-CA-N
3	С	502	3PO	PB-O3B-PG-O2G
4	А	503	SAM	CA-CB-CG-SD
4	D	503	SAM	C3'-C4'-C5'-SD
4	В	503	SAM	O-C-CA-CB
4	В	503	SAM	OXT-C-CA-CB
3	А	502	3PO	PB-O3A-PA-O5'

All (23) torsion outliers are listed below:

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	503	SAM	1	0
6	А	505	POP	2	0
2	С	501	ADN	1	0
2	D	501	ADN	1	0
4	D	503	SAM	4	0
3	В	502	3PO	1	0
4	В	503	SAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is



within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



































5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	385/407~(94%)	0.44	28 (7%) 15 13	16, 35, 62, 110	0
1	В	390/407~(95%)	0.49	33 (8%) 10 10	19, 35, 70, 124	0
1	С	386/407~(94%)	0.70	49 (12%) 3 3	25, 45, 76, 122	0
1	D	387/407~(95%)	0.66	35 (9%) 9 8	25, 47, 73, 105	0
All	All	1548/1628~(95%)	0.57	145 (9%) 8 7	16, 40, 73, 124	0

All (145) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	125	GLU	7.2
1	С	2	ALA	6.8
1	В	105	GLN	5.9
1	D	103	GLN	5.6
1	В	104	SER	5.5
1	D	2	ALA	5.3
1	А	103	GLN	4.9
1	В	122	ASP	4.6
1	С	210	ASP	4.5
1	А	2	ALA	4.5
1	В	407	ALA	4.4
1	С	236	ALA	4.4
1	В	406	LEU	4.3
1	С	190	GLN	4.3
1	С	4	PRO	4.2
1	С	237	THR	4.1
1	С	211	ARG	4.1
1	A	3	GLN	4.1
1	D	128	ARG	4.1
1	D	407	ALA	3.9
1	А	125	GLU	3.9



Mol	Chain	Res	Type	RSRZ
1	D	189	ALA	3.9
1	D	405	LYS	3.9
1	С	126	ASP	3.8
1	В	106	GLU	3.8
1	С	103	GLN	3.8
1	А	403	ALA	3.8
1	А	406	LEU	3.6
1	С	209	VAL	3.6
1	D	3	GLN	3.6
1	D	404	LEU	3.6
1	В	405	LYS	3.6
1	С	214	LEU	3.5
1	С	239	GLU	3.5
1	A	267	ILE	3.5
1	D	228	LYS	3.5
1	В	403	ALA	3.4
1	С	275	ALA	3.4
1	В	126	ASP	3.3
1	С	405	LYS	3.3
1	А	266	ILE	3.3
1	А	275	ALA	3.3
1	В	340	GLU	3.2
1	В	3	GLN	3.2
1	D	239	GLU	3.2
1	А	6	ALA	3.2
1	В	210	ASP	3.2
1	С	394	ILE	3.1
1	С	3	GLN	3.1
1	В	208	GLU	3.1
1	А	102	GLU	3.0
1	D	190	GLN	3.0
1	A	129	ALA	3.0
1	С	188	ASP	3.0
1	D	238	GLY	3.0
1	D	237	THR	3.0
1	В	123	VAL	3.0
1	D	234	ASP	3.0
1	D	236	ALA	2.9
1	D	125	GLU	2.9
1	D	266	ILE	2.9
1	В	402	ALA	2.9
1	В	397	VAL	2.9



Mol	Chain	Res	Type	RSRZ
1	В	266	ILE	2.8
1	D	173	PRO	2.8
1	В	103	GLN	2.8
1	С	407	ALA	2.8
1	С	232	ILE	2.7
1	А	349	ALA	2.7
1	С	208	GLU	2.7
1	С	233	GLU	2.7
1	В	4	PRO	2.7
1	А	5	THR	2.7
1	D	5	THR	2.7
1	А	405	LYS	2.6
1	А	209	VAL	2.6
1	А	208	GLU	2.6
1	С	276	ARG	2.5
1	D	323	GLY	2.5
1	В	404	LEU	2.5
1	С	49	VAL	2.5
1	С	250	PHE	2.5
1	D	401	ARG	2.5
1	А	192	ARG	2.5
1	D	195	HIS	2.5
1	D	340	GLU	2.5
1	В	270	THR	2.5
1	А	280	GLY	2.5
1	С	266	ILE	2.5
1	D	273	GLY	2.5
1	С	400	LEU	2.5
1	С	404	LEU	2.5
1	B	49	VAL	2.4
1	В	278	GLY	2.4
1	D	394	ILE	2.4
1	D	406	LEU	2.4
1	С	124	GLU	2.4
1	D	208	GLU	2.4
1	D	400	LEU	2.4
1	А	272	GLY	2.4
1	В	267	ILE	2.3
1	А	270	THR	2.3
1	С	274	MET	2.3
1	С	175	LEU	2.3
1	С	102	GLU	2.3



Mol	Chain	Res	Type	RSRZ
1	С	403	ALA	2.3
1	D	194	SER	2.3
1	А	268	VAL	2.3
1	В	124	GLU	2.3
1	С	92	ARG	2.3
1	D	146	GLU	2.3
1	А	399	GLU	2.2
1	В	341	GLY	2.2
1	С	136	LEU	2.2
1	А	295	ALA	2.2
1	С	251	ILE	2.2
1	В	207	PRO	2.2
1	В	401	ARG	2.2
1	D	42	SER	2.2
1	D	192	ARG	2.2
1	В	234	ASP	2.2
1	А	404	LEU	2.2
1	С	151	LEU	2.2
1	С	213	TRP	2.2
1	С	280	GLY	2.2
1	D	387	LEU	2.1
1	А	276	ARG	2.1
1	С	397	VAL	2.1
1	А	126	ASP	2.1
1	D	388	ASP	2.1
1	D	342	LEU	2.1
1	C	58	VAL	2.1
1	С	174	HIS	2.1
1	В	238	GLY	2.1
1	С	267	ILE	2.1
1	С	270	THR	2.1
1	В	346	GLN	2.1
1	С	273	GLY	2.1
1	В	276	ARG	2.0
1	С	192	ARG	2.0
1	С	128	ARG	2.0
1	С	364	ARG	2.0
1	В	248	GLY	2.0
1	A	62	ARG	2.0
1	С	264	ARG	2.0

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6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	ADN	С	501	19/19	0.86	0.21	35,51,61,61	0
2	ADN	А	501	19/19	0.88	0.17	28,37,41,42	0
2	ADN	D	501	19/19	0.88	0.18	33,41,44,47	0
7	MG	В	506	1/1	0.88	0.31	31,31,31,31	0
2	ADN	В	501	19/19	0.89	0.16	30,39,48,48	0
7	MG	D	504	1/1	0.90	0.24	43,43,43,43	0
3	3PO	В	502	13/13	0.91	0.18	27,32,47,54	0
4	SAM	А	503	27/27	0.91	0.18	35,42,64,66	0
8	K	А	508	1/1	0.91	0.15	60,60,60,60	0
7	MG	А	507	1/1	0.92	0.15	33,33,33,33	0
3	3PO	С	502	13/13	0.92	0.15	29,40,49,50	0
5	GOL	А	504	6/6	0.92	0.15	36,41,45,46	0
7	MG	D	505	1/1	0.92	0.19	26,26,26,26	0
6	POP	А	505	9/9	0.92	0.20	72,79,90,100	0
8	K	А	509	1/1	0.93	0.17	64,64,64,64	0
8	K	С	506	1/1	0.93	0.26	68,68,68,68	0
7	MG	А	506	1/1	0.94	0.25	29,29,29,29	0
4	SAM	D	503	27/27	0.94	0.20	33,37,61,62	0
4	SAM	В	503	27/27	0.95	0.17	31,40,72,78	0
7	MG	В	505	1/1	0.95	0.14	41,41,41,41	0
4	SAM	С	503	27/27	0.95	0.18	35,43,55,61	0
3	3PO	D	502	13/13	0.95	0.17	30,37,52,53	0
7	MG	С	504	1/1	0.96	0.23	33,33,33,33	0
5	GOL	В	504	6/6	0.96	0.13	32,37,39,40	0
3	3PO	А	502	13/13	0.96	0.14	28,32,45,51	0
7	MG	С	505	1/1	0.97	0.19	43,43,43,43	0
8	K	D	506	1/1	0.97	0.13	69,69,69,69	0



The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.































































6.5 Other polymers (i)

There are no such residues in this entry.

